# Nayara D Coutinho

List of Publications by Year
in descending order



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|---|---|---|---|
| 21 papers | 381 citations | 1040056 9 h-index | 794594 19 g-index |
| 21 all docs | 21 docs citations | 21 times ranked | 312 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Temperature Dependence of Rate Processes Beyond Arrhenius and Eyring: Activation and Transitivity. Frontiers in Chemistry, 2019, 7, 380. | 3.6 | 69 |
| 2 | Stereodynamical Origin of Anti-Arrhenius Kinetics: Negative Activation Energy and Roaming for a Four-Atom Reaction. Journal of Physical Chemistry Letters, 2015, 6, 1553-1558. | 4.6 | 63 |
| 3 | Kinetics of low-temperature transitions and a reaction rate theory from non-equilibrium distributions. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2017, 375, 20160201. | 3.4 | 57 |
| 4 | Stereodirectional Origin of anti-Arrhenius Kinetics for a Tetraatomic Hydrogen Exchange Reaction: Bornâ€“Oppenheimer Molecular Dynamics for OH + HBr. Journal of Physical Chemistry A, 2016, 120, 5408-5417. | 2.5 | 30 |
| 5 | A novel assessment of the role of the methyl radical and water formation channel in the CH<sub>3</sub>OH + H reaction. Physical Chemistry Chemical Physics, 2017, 19, 24467-24477. | 2.8 | 22 |
| 6 | Kinetics of the OH+HClâ†'H<sub>2</sub>O+Cl reaction: Rate determining roles of stereodynamics and roaming and of quantum tunneling. Journal of Computational Chemistry, 2018, 39, 2508-2516. | 3.3 | 22 |
| 7 | Description of the effect of temperature on food systems using the deformed Arrhenius rate law: deviations from linearity in logarithmic plots vs. inverse temperature. Rendiconti Lincei, 2015, 26, 141-149. | 2.2 | 18 |
| 8 | From statistical thermodynamics to molecular kinetics: the change, the chance and the choice. Rendiconti Lincei, 2018, 29, 787-802. | 2.2 | 18 |
| 9 | â€œTransitivityâ€• A Code for Computing Kinetic and Related Parameters in Chemical Transformations and Transport Phenomena. Molecules, 2019, 24, 3478. | 3.8 | 18 |
| 10 | From the Kinetic Theory of Gases to the Kinetics of Rate Processes: On the Verge of the Thermodynamic and Kinetic Limits. Molecules, 2020, 25, 2098. | 3.8 | 10 |
| 11 | Topography of the free energy landscape of Claisenâ€“Schmidt condensation: solvent and temperature effects on the rate-controlling step. Physical Chemistry Chemical Physics, 2021, 23, 6738-6745. | 2.8 | 10 |
| 12 | Description of deviations from Arrhenius behavior in chemical kinetics and materials science. AIP Conference Proceedings, 2016, , . | 0.4 | 9 |
| 13 | Aminoâ€“Imino Tautomerism in the Salt Formation of Albendazole: Hydrobromide and Nitrate Salts. Crystal Growth and Design, 2021, 21, 1122-1135. | 3.0 | 9 |
| 14 | Temperature dependence of rate constants for the H(D) + CH4 reaction in gas and aqueous phase: deformed Transition-State Theory study including quantum tunneling and diffusion effects. Structural Chemistry, 2020, 31, 609-617. | 2.0 | 8 |
| 15 | Effect of the Methanol Molecule on the Stabilization of C<sub>18</sub>H<sub>18</sub>O<sub>4</sub> Crystal: Combined Theoretical and Structural Investigation. Journal of Physical Chemistry A, 2014, 118, 10048-10056. | 2.5 | 5 |
| 16 | Nucleophilic substitution vs elimination reaction of bisulfide ions with substituted methanes: exploration of chiral selectivity by stereodirectional first-principles dynamics and transition state theory. Journal of Molecular Modeling, 2019, 25, 227. | 1.8 | 5 |
| 17 | First-Principles Molecular Dynamics and Computed Rate Constants for the Series of OH-HX Reactions (Xâ€‰=â€‰H or the Halogens): Non-Arrhenius Kinetics, Stereodynamics and Quantum Tunnel. Lecture Notes in Computer Science, 2018, , 605-623. | 1.3 | 3 |
| 18 | The $$ {mathbf{HI}},varvec{ + },{mathbf{OH}}, o ,{mathbf{H}}_{{mathbf{2}}} {mathbf{O}}, + ,{mathbf{I}} $$ HI + OH â†' H 2 O + I Reaction by First-Principles Molecular Dynamics: Stereodirectional and anti-Arrhenius Kinetics. Lecture Notes in Computer Science, 2017, , 297-313. | 1.3 | 3 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | The Increase of the Reactivity of Molecular Hydrogen with Hydroxyl Radical from the Gas Phase versus an Aqueous Environment: Quantum Chemistry and Transition State-Theory Calculations. Lecture Notes in Computer Science, 2019, , 450-459. | 1.3 | 1 |
| 20 | Reply to the â€˜Comment on â€œTopography of the Free Energy Landscape on the Claisenâ€“Schmidt Condensation: Solvent and Temperature Effect in the Rate-Controlling Stepâ€â€™ by N. D. Coutinho, H. G. Machado, V. H. Carvalho-Silva and W. A. da Silva, Phys. Chem. Chem. Phys., 2021, 23, 6738. Physical Chemistry Chemical Physics, 2021, 23, 22202-22206. | 2.8 | 1 |
| 21 | Rate constants and first-principles trajectories for attack at tetrahedral carbon: Role of molecular orientation on chiral selectivity. AIP Conference Proceedings, 2019, , . | 0.4 | 0 |